Enumerating Acyclic Orientations

Research Capstone Thesis

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1 Introduction

An *acyclic orientation* (AO) on a graph is an assignment of direction to each of the edges without introducing a directed cycle. An *acyclic unique sink orientation* (AUSO) is an AO in which only one vertex has all edges directed inward; that is, all other vertices have at least one edge leaving the vertex.

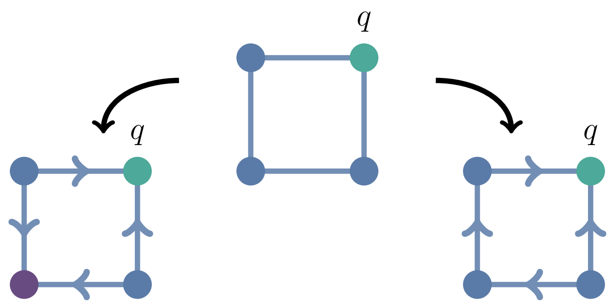


Figure 1: Two AOs of a graph. The left is not an AUSO while the right is, with unique sink q

AOs have classically been of interest to mathematicians in combinatorics and graph theory for the deep connections they share with other well-known graph properties like the chromatic and Tutte polynomials, spanning trees, etc. [Sta73, GZ83, GV05, GS00]. Additionally, in computer science, AOs and AUSOs both lie in the gap in our understanding regarding tractability of enumeration and sampling. As Tutte polynomial evaluations, enumerating them exactly is known to be hard [Lin86]. It is still not known, however, if they admit efficient approximation algorithms [GJ12].

More recently, interest in these graph properties has expanded to other fields as they have become useful for modeling in biology and statistical physics. In the biology community there is interest in the behavior of so-called *branched polymers*. In particular, it is useful to know what a randomly selected branched polymer looks like. These branched polymers can be modeled with graphs, and their behavior under randomness can be understood through the counting of AUSOs [KW09] (equivalently, spanning trees with no broken circuit [GV05]). Another source of interest in counting acyclic orientations comes from statistical physics through their connection to the *Ursell function* [HPR18]. The Ursell function of a graph G with edge set E is

$$\phi(G) = \sum_{\substack{A \subseteq E \\ A \text{ spanning, connected}}} (-1)^{|A|}.$$

It is NP-hard to compute in general, but can be easily computed knowing the number of AUSOs on G.

For a graph G, denote by $\mathcal{A}(G)$ and $\mathcal{A}(G, q)$ the set of AOs and AUSOs with sink at chosen vertex q respectively. This thesis addresses questions relating to the above interests in AOs and AUSOs. Specifically, we consider three broad types of questions:

- **Enumerative/bijective**: because of the intractability of computing $|\mathcal{A}(G)|$ and $|\mathcal{A}(G,q)|$, we focus on computing these values for some specific families of graphs.

- **Extremal**: we consider the problem of determining which graph(s) among those with a fixed number of vertices and edges maximize the number of AOs.

- **Algorithmic**: we investigate a Markov chain Monte Carlo approach to approximate sampling and counting of AOs.

We begin in Section 2 with a brief review of background and the relevant literature. We then look at counting AUSOs of $m \times n$ grid graphs, $G_{m,n}$ in Section 3. Such graphs are common in statistical physics models, and so are a natural family of graphs to consider. Moreover, the $2 \times n$ grid $G_{2,n}$ has a simple answer. We find a recurrence and formula for AUSOs of $3 \times n$ grids.

In Section 4, we shift focus to complete bipartite and multipartite graphs. Cameron, Glass, and Schumacher found an explicit formula for the number of AOs of any complete bipartite graph [CGS14], and asked if a similar formula could be given for any complete multipartite graph. In this work we provide such a formula. Our techniques are easily altered to give an explicit formula for the number of AUSOs with sink q for the same family of graphs. In this section, we also provide a simple and natural bijection between the set of AUSOs of complete *bipartite* graphs and permutations with a prescribed *excedance set*. In particular, this connects two combinatorial structures which were previously not known to be related.

In Section 5, we give a partial extremal result concerning the graph(s) which maximize the number of AOs for a fixed number of vertices and edges. A Turán graph is a complete multipartite graph on n vertices in which each part has size $\lceil \frac{n}{r} \rceil$ or $\lfloor \frac{n}{r} \rfloor$ for some r. Cameron, Glass, and Schumacher gave a conjecture that the Turán graph is a maximizer, when it exists for a given number of vertices and edges [CGS14]. We confirm this conjecture for a specialized case: specifically, when the number m of edges and n vertices satisfies $m \geqslant \binom{n}{2} - \lfloor \frac{n}{2} \rfloor$.

In Section 6, we consider the problem for an algorithmic perspective. In particular, we investigate the technique of Markov chain Monte Carlo (MCMC) methods for efficiently sampling a random acyclic orientation.

Finally, in Section 7, we make some concluding remarks on our work and future directions.

The results of Sections 3, 4, and 5 are being prepared by the Arvind Ayyer, the author, and Prasad Tetali [AHT20]. The subject of Section 6.2 is a work in progress by the author, Prasad Tetali, and Josephine Yu [HTY20].

2 Background and Literature Review

2.1 Acyclic orientations

The study of acyclic orientations began with their connections to colorings and the chromatic polynomial. Because of the many deep connections subsequently discovered, interest in the topic has grown in the mathematical community to gain a deeper understanding of these objects.

We begin with the relevant terminology. In particular, letting G be a (simple) graph (as usual, a network of vertices connected by edges), we define

Definition 2.1 (Orientation)**.** Given a graph $G = (V, E)$, an **orientation** of G is an assignment of a direction to each edge in E. We say the orientation is **acyclic** if there are no directed cycles. We say the orientation has a fixed **unique sink** $q \in V$ if q is the only vertex in the orientation with out-degree 0.

Denote by $\mathcal{A}(G)$ the set of all AOs of G. For some fixed vertex $q \in V$, denote by $\mathcal{A}(G, q)$ the set of AUSOs of G for which q is the unique sink. Also, denote by $\mathcal{A}(G, \cdot)$ the set of all AUSOs of G with any sink vertex. That is, $\mathcal{A}(G, \cdot) = \bigcup_q \mathcal{A}(G, q)$. Closely connected to the sizes of these sets are the chromatic and Tutte polynomials:

Definition 2.2 (Chromatic Polynomial)**.** For graph G, the **chromatic polynomial** $\chi_G(\lambda)$ is the function which gives the number of ways to **properly color** the vertices of G with λ colors (originally introduced for general graphs by Whitney in [Whi32], along with proof that $\chi_G(\lambda)$ is a polynomial).

Definition 2.3 (Tutte Polynomial)**.** For a graph $G = (V, E)$, the **Tutte polynomial** is the two-variate polynomial

$$T_G(x, y) = \sum_{A \subseteq E} (x - 1)^{k(A) - k(E)} (y - 1)^{k(A) + |A| - |V|}$$

where, for $S \subseteq E$, $k(S)$ is the number of connected components of the graph $G' = (V, S)$ (introduced by Tutte in [Tut54]).

Following the discovery of these graph polynomials, a connection between acyclic orientations and the chromatic polynomial was discovered by Stanley [Sta73]. In particular

$$|\mathcal{A}(G)| = (-1)^{|V|} \chi_G(-1) = |\chi_G(-1)|$$

Stanley proved this using the classical deletion-contraction recurrence of the chromatic polynomial on graphs. That is, for a graph G, say $G - e$ is the graph resulting from deleting an edge, and G/e is the graph resulting from contracting the two endpoints of an edge into a single vertex. Then,

$$\chi_G(\lambda) = \chi_{G-e}(\lambda) - \chi_{G/e}(\lambda)$$

In fact, it is easily shown that the chromatic polynomial is uniquely defined by this recurrence, along with the two facts

- $\chi_{G_0}(\lambda) = \lambda$ where G_0 is the graph on one vertex.
- $\chi_{G \cup H}(\lambda) = \chi_G(\lambda) \cdot \chi_H(\lambda)$ for any two graph G and H, and their disjoint union $G \cup H$.

Stanley used this characterization to show that a function defined in terms of acyclic orientations is equal to $(-1)^{|V|}\chi_G(\lambda)$, from which the result immediately follows.

Building off of this work, Greene and Zaslavsky [GZ83], and Gebhard and Sagan [GS00] gave various proofs that, letting $a_1(p)$ be the coefficient of the linear term of polynomial p,

$$|\mathcal{A}(G, q)| = |a_1(\chi_G)|$$

in particular showing the surprising fact that $|\mathcal{A}(G, q)|$ is invariant of the choice of $q \in V$. In particular, for a graph on n vertices, $|\mathcal{A}(G, \cdot)| = n \cdot |\mathcal{A}(G, q)|$.

Gebhard and Sagan's work gives three proofs showing this equivalence: pure induction on the number of edges of G, a technique using noncommutative symmetric functions, and an algorithmic bijection. The inductive proof makes use of the deletion-contraction recurrence of the chromatic polynomial to find the behavior of the linear term. The algorithmic proof builds off of Whitney's Broken Circuit Theorem [Whi32].

There have been several bijective proofs of equivalence between $|\mathcal{A}(G, q)|$ and other structures, such as spanning trees with no broken circuit

Definition 2.4 (Broken Circuit)**.** For a graph G and total ordering σ of the edges, a **broken circuit** with respect to σ is a cycle minus one edge such that the missing edge is maximal in the cycle.

For some edge ordering σ, denote by $\mathcal{T}(G, \sigma)$ the set of spanning trees containing no broken circuit. The size of $\mathcal{T}(G, \sigma)$ is closely related to the $\chi_G(\lambda)$ by the classical result of Whitney, now called the Broken Circuit Theorem [Whi32].

Definition 2.1.1 (Activity)**.** Let T be a spanning tree of graph G, and let $e \in T$ be an edge. Removing e from T separates it into two sets S and $V \setminus S$ of vertices. The **fundamental cocycle** of e is the set of edges spanning the cut $(S, V \setminus S)$.

For an edge $e \notin T$, the **fundamental cycle** is the unique cycle induced by adding e to T.

For a spanning tree T, and a linear ordering σ on all of the edges of G, the **internal activity** of T is the number of edges $e \in T$ smallest in their fundamental cocycle, while the **external activity** of T is the number of edges $e \notin T$ smallest in their fundamental cycle.

Further connections between the size of $\mathcal{T}(G, \sigma)$ and AUSOs were shown by Gioan and Las

Vergnas [GV05]. The paper gives an algorithmic bijection between the number of spanning trees with internal activity 1, external activity 0 and the number of acyclic orientations with unique adjacent source and sink. They then give a more general "activity preserving" bijection between spanning trees and certain orientations, which extends to a bijection between spanning trees with no broken circuit (those with 0 external activity) and acyclic orientations with a unique sink.

Finally, the work of Benson, Chakrabarti, and Tetali bijectively relates all of these graph properties to another property called G-parking functions [BCT10]. They show the number of maximal G-parking functions is equivalent to many of the same properties relating to $\mathcal{A}(G,q)$. In summary, for any graph $G=(V,E)$, any $q \in V$, and any edge ordering σ, the following are all equal:

- The number of maximum G-parking functions with respect to q.
- $|\mathcal{A}(G,q)|$.
- $|\mathcal{T}(G,\sigma)|$.
- $|a_1(\chi_G)|$.
- $|T_G(1,0)|$.

2.2 Exact Enumeration

It was shown by Linial that counting the number of acyclic orientations $|\mathcal{A}(G)|$ for a general graph is $\#P$-complete [Lin86]. He reduced the computation of the chromatic polynomial of a graph to enumerating acyclic orientations. Using the connection between $|\mathcal{A}(G)|$ and $\chi_G(-1)$, he uses slight alterations of the graph to find enough evaluations of χ_G to compute its coefficients.

For any graph G, consider the join $G+v$ with some singleton vertex (that is, the graph on vertex set $V \cup \{v\}$ and edge set $E \cup \{(v,u) \mid u \in V\}$). Observe that $|\mathcal{A}(G)| = |\mathcal{A}(G+v,v)|$ by the obvious bijection. This reduction shows that counting $|\mathcal{A}(G,q)|$ is also $\#P$-complete in general (as it is clearly in $\#P$). Therefore, the best direct enumeration results we can hope for involve specific families of graphs.

Kahale and Schulman give bounds on $|\mathcal{A}(Q_d)|$, where Q_d is the d-dimensional hypercube graph [KS96]. Specifically they use the probabilistic method for a lower bound, and they relate AOs with the spectrum of the Laplacian matrix for an upper bound, showing that

$$\left(\frac{d}{2}+1\right)^{2^d} \leqslant |\mathcal{A}(Q_d)| \leqslant (d+1)^{2^d}.$$

Similarly, Matoušek found a lower bound on the number of AUSOs for Q_d [Mat06]. He wrote this bound in terms of all AUSOs, without specifying a single sink vertex. But, recall that for graphs on n vertices, $|\mathcal{A}(G,\cdot)| = n \cdot |\mathcal{A}(G,q)|$. Using a simple induction, Moutšek showed

$$2^{2^{d-1}} \leqslant |\mathcal{A}(Q_d,\cdot)| \leqslant (d+1)^{2^d}$$

where the upper bound comes from the Kahale and Schulman bound on all AOs.

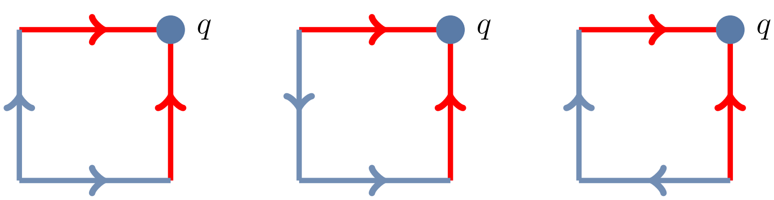
Concerning work in direct enumeration of a specific family, Cameron, Glass, and Schumacher gave a simple formula for the number of acyclic orientations for the complete bipartite graphs K_{n_1,n_2}. They show

$$\mathcal{A}(K_{n_1,n_2}) = \sum_{k=1}^{\min(n_1,n_2)+1} ((k-1)!)^2 S(n_1+1,k)S(n_2+1,k)$$

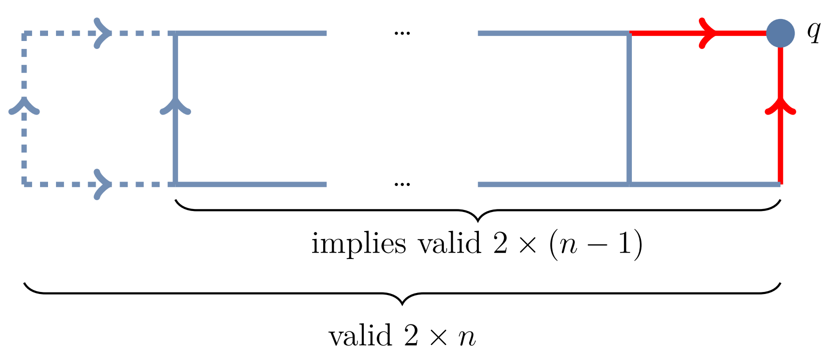
where $S(n,k)$ is the Stirling number of the second kind. This is achieved by finding an equivalent representation of acyclic orientations in terms of a totally ordered list of vertices, with structure from the two partitions. They ask if a similar technique could be used for complete multipartite graphs.

3 Grid Graphs

The number of AUSOs with fixed sink vertex q for $2 \times n$ grids is 3^{n-1}. For example, for the 2×2 grid with sink q:



This can be easily counted inductively by proving that, for any *valid* (acyclic with unique sink) $2 \times n$ orientation, the $2 \times (n-1)$ grid subgraph containing q must also be valid:



Then it is an easy task to show that each valid $2 \times (n-1)$ orientation can be made into exactly 3 valid $2 \times n$ orientations by "tacking on" another two vertices to the left. Since the 2×1 grid has 1 valid orientation, this gives 3^{n-1} valid for the $2 \times n$.

Theorem 3.1. The number of AUSOs with fixed sink q of the $3 \times n$ grid is given by

$$\frac{1}{154}\left[(7+3\sqrt{14})(5+\sqrt{14})^n + (7-3\sqrt{14})(5-\sqrt{14})^n\right]$$

Proof. The proof works similarly to the $2 \times n$ proof, but we have to take cases, and also have to account for valid $3 \times n$ orientations which are generated by an *invalid* $3 \times (n-1)$ (this only happens in the $3 \times n$ case, not the $2 \times n$).

We will break into cases, and find a recurrence to count the number of each case for the $3 \times n$ grid based on the number for the $3 \times (n-1)$ grid. The cases are:

Let a_n, b_n, c_n, d_n be the number of valid cases of A, B, C, and D respectively for the $3 \times n$ grid. The number we are trying to compute is $a_n + b_n + c_n + d_n$.

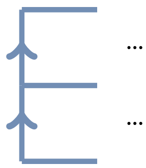


Figure 2: Case A

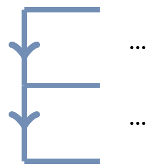


Figure 3: Case B

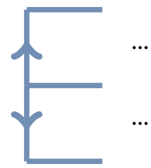


Figure 4: Case C

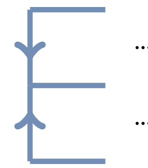
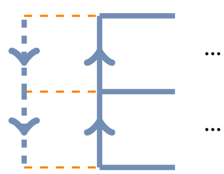
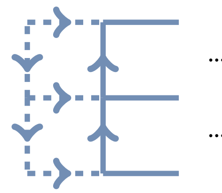


Figure 5: Case D

To begin finding the recurrence, we can (somewhat painstakingly) count the number of valid $3 \times n$ cases which are generated by each valid $3 \times (n-1)$ case. For example, the number of valid $3 \times n$ case B's which are generated by a valid $3 \times (n-1)$ case A is only 1:



can only be valid if



Notice that any other orientation of the orange dashed edges would cause either a sink in the bottom left vertex, or a cycle. Notice also that, so long as the $3 \times (n-1)$ is valid, then the generated $3 \times n$ will also be valid.

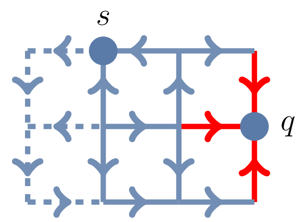
In this way, we can count the number of valid $3 \times n$ of each case generated by valid $3 \times (n-1)$ of each case (in the above example, we showed that each of the b_{n-1} valid $3 \times (n-1)$ case B's contributes just 1 valid $3 \times n$ case A):

$$\begin{aligned}
\#\left[\text{Valid } 3 \times n \text{ case A's generated by valid } 3 \times (n-1)\right] &= 4a_{n-1} + b_{n-1} + 3c_{n-1} + 2d_{n-1} \\
\#\left[\text{Valid } 3 \times n \text{ case B's generated by valid } 3 \times (n-1)\right] &= a_{n-1} + 4b_{n-1} + 3c_{n-1} + 2d_{n-1} \\
\#\left[\text{Valid } 3 \times n \text{ case C's generated by valid } 3 \times (n-1)\right] &= a_{n-1} + b_{n-1} + 2c_{n-1} + d_{n-1} \\
\#\left[\text{Valid } 3 \times n \text{ case D's generated by valid } 3 \times (n-1)\right] &= 2a_{n-1} + 2b_{n-1} + c_{n-1} + 4d_{n-1}
\end{aligned}$$

Note that the left hand side of these identities should *not* necessarily be a_n, b_n, c_n, and d_n respectively, as there are potentially some valid $3 \times n$ cases generated by an *invalid* $3 \times (n-1)$.

It can be shown rather easily in the counting process above that, for any valid $3 \times n$ generated by a case A, B, or D $3 \times (n-1)$, it must be the case that the $3 \times (n-1)$ is also valid (this can be determined by inspection of the three leftmost vertices in the $3 \times (n-1)$: if any of them are allowed to be a sink in the $3 \times (n-1)$, it would cause a sink in the generated $3 \times n$, a contradiction since we assumed this was valid).

On the other hand, a valid $3 \times n$ *can* be generated by an invalid case C $3 \times (n-1)$. For example:



Notice that vertex s is a sink in the 3×3 (making it invalid), but the 3×4 is a valid orientation.

Fortunately, there are only two such cases for us to count (we may determine that there are only two in the counting process above):

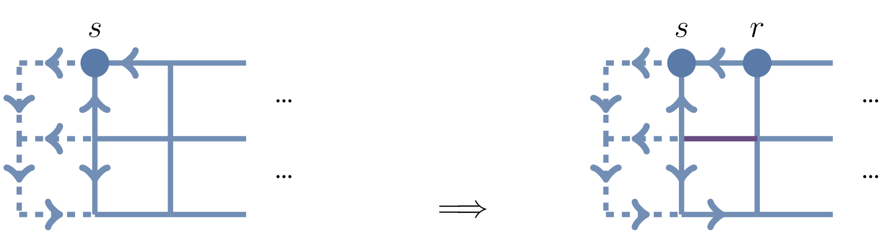
In particular, only $3 \times n$ cases A and B can be generated by an invalid $3 \times (n-1)$. So we may now write:

$$\begin{aligned}
a_n &= 4a_{n-1} + b_{n-1} + 3c_{n-1} + 2d_{n-1} + \#[\text{case A generated by invalid } 3 \times (n-1) \text{ case C}] \\
b_n &= a_{n-1} + 4b_{n-1} + 3c_{n-1} + 2d_{n-1} + \#[\text{case B generated by invalid } 3 \times (n-1) \text{ case C}] \\
c_n &= a_{n-1} + b_{n-1} + 2c_{n-1} + d_{n-1} \\
d_n &= 2a_{n-1} + 2b_{n-1} + c_{n-1} + 4d_{n-1}
\end{aligned}$$

At this point, we use symmetry to simplify this by writing $e_n = a_n + b_n$, and also letting s_{n-1} be the number of valid $3 \times n$ case A or B generated by an invalid $3 \times (n-1)$ case C. So,

$$\begin{aligned}
e_n &= 5e_{n-1} + 6c_{n-1} + 4d_{n-1} + s_{n-1} \\
c_n &= e_{n-1} + 2c_{n-1} + d_{n-1} \\
d_n &= 2e_{n-1} + c_{n-1} + 4d_{n-1} \\
s_n &= ?
\end{aligned}$$

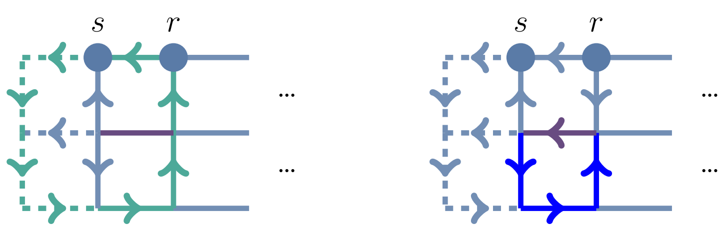
Now we only need to find a recurrence to count s_n. We actually count half of s_{n-1} by focusing on the valid $3 \times n$ case B's generated by invalid $3 \times (n-1)$ case C's (but by symmetry the number of case A's generated this way is the same). Since we require the $3 \times (n-1)$ be invalid, we want vertex s (from the above example) to be a sink in the $3 \times (n-1)$, so we have



Now we split into two cases

- The $3 \times (n-2)$ is invalid. It can only be invalid if vertex r is a sink (in the $3 \times (n-2)$), in which case the $3 \times (n-2)$ must be a case C to avoid a cycle. This is simply $\frac{s_{n-2}}{2}$, but then we have 2 choices for the purple edge, so this case has s_{n-2} total ways.

- The $3 \times (n-2)$ is valid. Not all valid $3 \times (n-2)$ work however: a case A would form a large cycle in the left 3×3 vertices (in green below), and a case D would force a choice for the purple edge to avoid a cycle (blue below):



  Other than these two choices, all other valid $3 \times (n-2)$ work, so we get (with the choice of the purple edge):

$$2(b_{n-2} + c_{n-2}) + d_{n-2} = 2\left(\frac{e_{n-2}}{2} + c_{n-2}\right) + d_{n-2} = e_{n-2} + 2c_{n-2} + d_{n-2} = c_{n-1}$$

Thus, we have found

$$\frac{s_{n-1}}{2} = c_{n-1} + s_{n-2} \implies s_n = 2c_n + 2s_{n-1} = 2e_{n-1} + 4c_{n-1} + 2d_{n-1} + 2s_{n-1}$$

which in total gives us a final recurrence for all $n \geqslant 1$ (in matrix form):

$$\begin{bmatrix} e_n \\ c_n \\ d_n \\ s_n \end{bmatrix} = \begin{bmatrix} 5 & 6 & 4 & 1 \\ 1 & 2 & 1 & 0 \\ 2 & 1 & 4 & 0 \\ 2 & 4 & 2 & 2 \end{bmatrix}^{n-1} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

since the 3×1 clearly has exactly one case D. Now, to count the total, let $t_n = e_n + c_n + d_n$, and get the recurrence

$$\begin{bmatrix} t_n \\ e_n \\ c_n \\ d_n \\ s_n \end{bmatrix} = \begin{bmatrix} 0 & 8 & 9 & 9 & 1 \\ 0 & 5 & 6 & 4 & 1 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 2 & 1 & 4 & 0 \\ 0 & 2 & 4 & 2 & 2 \end{bmatrix}^{n-1} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

Solving this for t_n yields

$$t_n = \frac{1}{154}\left[(7 + 3\sqrt{14})(5 + \sqrt{14})^n + (7 - 3\sqrt{14})(5 - \sqrt{14})^n\right] \qquad \square$$

Note that the above recurrence can be simplified to a second order linear recurrence

$$t_n = 10t_{n-1} - 11t_{n-2}$$

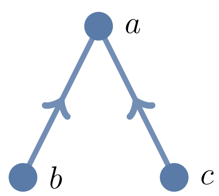
though it appears difficult to prove this directly. We can also compute the initial conditions for larger (e.g. $4 \times n$ and $5 \times n$) cases, and attempt to determine linear recurrences for these as well. Unfortunately, it appears that the order of the recurrence increases in a nontrivial way (3rd order for $4 \times n$, and 7th order for $5 \times n$). So, there maybe not be a simple way to write down a general answer for the $m \times n$ grid.

4 AOs of Complete Multipartite Graphs

We now focus on complete bipartite and multipartite graphs. The discussion will be made easier by considering *topological sorts* of the vertices of an acyclic orientation.

Definition 4.1 (Topological Sort)**.** Given a directed acyclic graph (e.g., an acyclic orientation of any graph), a **topological sort** of the vertices is a total ordering τ on the vertices such that for every edge $e = (u, v)$ (i.e. with direction $u \to v$), then $\tau(u) < \tau(v)$. We will often say that an *undirected* graph G has topological sort τ if there is an AO on G with topological sort τ.

Example 4.1. Notice that a given directed acyclic graph can have multiple topological sorts. For example,



$$\tau_1 = b, c, a \quad \text{and} \quad \tau_2 = c, b, a$$

Lemma 4.1. If K is a complete multipartite graph with vertices labeled $1, 2, \ldots, n$, then there is a bijection between AOs of K and the topological sorts of K in which adjacent and incomparable vertices are in increasing numerical order. Call such topological sorts **canonical** topological sorts of K.

Proof. It is immediate that any topological sort of the vertices of K uniquely defines an AO on K.

Given an AO of K, two vertices are incomparable if and only if they are in the same vertex set, and have identical in/out-neighborhoods (otherwise there would be a directed path from one to the other). Thus, we may partition all vertices in equivalence/incomparability classes. Any topological sort is a particular ordering of these classes, paired with any orderings within each class. Simply ordering each class by σ gives the unique topological sort following the desired condition. $\square$

Definition 4.2. For a permutation $\sigma \in S_k$, the **excedance set** is the set of elements whose position (strictly) exceeds its own value:

$$\text{ex}(\sigma) = \big\{ i \in \{1, \ldots, k\} \,\big|\, \sigma(i) > i \big\}$$

For $m, n > 0$, denote by $T(m+n, m)$ the set of permutations of $\{1, \ldots, m+n\}$ with excedance set $\{1, \ldots, m\}$:

$$T(m+n, m) = \big\{ \sigma \in S_{m+n} \,\big|\, \text{ex}(\sigma) = \{1, \ldots, m\} \big\}$$

Example 4.2. For a permutation σ, it will be convenient to consider the (disjoint) cycle decomposition $\sigma = \sigma_1 \ldots \sigma_k$. It is not hard to see that $\sigma \in T(m+n, m)$ if and only if each individual cycle satisfies that if $a \to b$, then

- $a < b$ if and only if $a \in \{1, \dots, m\}$ (since $\sigma(a) = b > a$).

- $a \geqslant b$ if and only if $a \in \{m+1, \dots, m+n\}$.

For example, if $m = 4$, $n = 6$, then we may consider the permutation $\sigma = (27)(138645)$. Both cycles follow the the above property: (27) increases only after 2, and (138645) increases after 1, 3, and 4. And indeed, $\mathrm{ex}(\sigma) = \{1, 2, 3, 4\}$.

While discussing the complete bipartite graph $K_{m,n}$, we refer to the 'Left' vertex set containing m vertices as $L = \{1, \dots, m\}$, and the 'Right' containing n vertices as $R = \{m+1, \dots, m+n\}$.

Denote by $t_{m,n}$ the number of acyclic orientations with a fixed unique sink vertex of $K_{m,n}$ (recall the choice of sink vertex doesn't matter). Denote by $G(m,n)$ the set of acyclic orientations of $K_{m,n}$ in which there are no sinks in L (the set containing m vertices). By simply adding a vertex to L to get $K_{m+1,n}$ and demanding this vertex be a sink, we maintain the acyclic property, and the added vertex becomes the unique sink. Removing the vertex gives the inverse, and the resulting bijection shows

$$|G(m,n)| = t_{m+1,n}$$

4.1 A Bijection between AUSOs and Permutations

We define a bijection between AUSOs of $K_{m+1,n}$ and $T(m+n, m)$. We use the discussion above to write the bijection in terms of the cycle decomposition of permutations in $T(m+n, m)$ and orientations in $G(m,n)$ (those with no sink in L).

Let $f\colon T(m+n,m) \to G(m,n)$ be defined as follows. For $\sigma \in T(m+n,m)$, construct $f(\sigma)$ by:

1. Consider the cycle decomposition of σ. Write each cycle such that its least element appears first.

2. Order the cycles, relative to each other, from right to left by least element (disjoint cycles commute).

3. Remove the parentheses around the cycle decomposition as written in step 2, and consider the resulting sequence of vertices as a topological sort of an orientation on $K_{m,n}$ (notice a topological sort uniquely determines the orientations of all edges).

Example 4.1.1. Suppose $m = 4$, $n = 5$, and we are given the permutation

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 3 & 9 & 6 & 7 & 5 & 2 & 4 & 8 & 1 \end{pmatrix} = (13629)(47)(5)(8)$$

It is easy to verify that $\sigma \in T(9,4)$ (notice $\mathrm{ex}(\sigma) = \{1, \dots, 4\}$). To construct $f(\sigma)$ notice that each cycle is already written according to step 1. Step 2 yields

$$(\underline{8})(\underline{5})(\underline{4}7)(\underline{1}3629)$$

and finally, step 3 gives the topological sort: $8, 5, 4, 7, 1, 3, 6, 2, 9$, with the resulting orientation being acyclic and containing no sink in $L = \{1, 2, 3, 4\}$. We can check this by seeing that the last vertex in the topological sort is in R, so no vertex in L can be a sink.

Lemma 4.1.1. The function f indeed maps into $G(m, n)$.

Proof. Consider any permutation σ. Since $f(\sigma)$ is an orientation determined by a topological sort, it must be acyclic.

Write σ according to step 2 (of the description of f) as $\sigma = \sigma_1 \dots \sigma_k$. The rightmost vertex v in the topological sort $f(\sigma)$ will be the final term in the cycle $\sigma_k = (1 \dots v)$. In particular, $\sigma(v) = 1$ and since 1 is the least element, $\sigma(v) \leqslant v$. Therefore

$$v \in \overline{\mathrm{ex}(\sigma)} = \{m + 1, \dots, m + n\} = R$$

Since v is the rightmost term of the topological sort, it is a sink. Since it is in R, it has all vertices in L as a neighbor, so no vertex in L can be a sink. □

Theorem 4.1.2. The function f is a bijection.

Proof. We prove this by giving the inverse function. Given an acyclic orientation $\mathcal{O} \in G(m, n)$, construct $f^{-1}(\mathcal{O})$ as follows:

Since $\mathcal{O}$ is acyclic, it has a topological sort. But it may not be unique, as there could be vertices u, v either both in L or both in R which are whose positions could be swapped (they are equivalent). We designate a unique topological sort by specifying that whenever $u < v$, with u and v equivalent:

- if $u, v \in L$, then u appears before v in the topological sort.
- if $u, v \in R$, then u appears after v in the topological sort.

This defines a unique topological sort $v_1, \dots, v_{m+n}$, and there is a unique way to insert parentheses into the sequence to make it into a cycle decomposition written as specified in step 2 of the description of f. i.e. the rightmost cycle contains 1 and all elements to its right, the next cycle contains the next smallest unused element and all unused elements to its right, etc.

To see that the resulting permutation $f^{-1}(\mathcal{O})$ has exceedance set L, notice that our tie-breaking strategy and the fact that all elements of L are less than those of R ensures the following conditions:

1. In the topological sort, $v_i < v_{i+1}$ if and only if $v_i \in L$

2. Because we inserted parentheses by choosing the next smallest unused element, every cycle $(v_i \dots v_{i+k})$ must have either $v_i \in L$ and $v_{i+k} > v_i$, or $v_i \in R$ and $v_{i+k} = v_i$ (that is, $k = 0$)

These two conditions ensure that in every cycle $(v_i, \dots, v_{i+k})$, we have $v_j \to v_{j+1}$ increases if and only if $v_j \in L$. Thus, the excedance set of the permutation is L, as desired. $\square$

Example 4.1.2. As an example of f^{-1}, we reverse the example we did while defining f (recall $m = 4$, $n = 5$). We could start with an orientation which has topological sort $5, 8, 4, 7, 3, 1, 6, 2, 9$ (notice no sink in L).

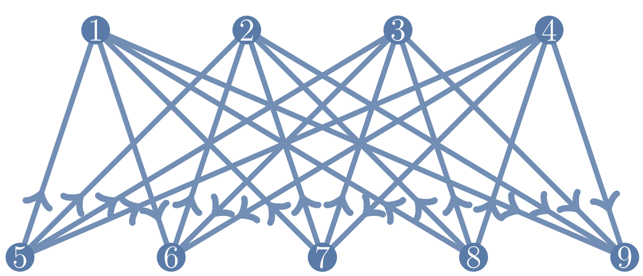
Notice that in this orientation, vertices $5, 8 \in R$ are equivalent, as well as vertices $1, 3 \in L$. So, using the tie-breaking strategy, we get the unique topological sort:

$$8, 5, 4, 7, 1, 3, 6, 2, 9$$

Now, we insert parentheses first left of 1, then left of 4, then 5, then 8:

$$f^{-1}(\mathcal{O}) = (8)(5)(47)(13629)$$

And notice that for this permutation, $f^{-1}(f(\sigma)) = \sigma$, as we expected.



$8, 5, 4, 7, 1, 3, 6, 2, 9 \to (8)(5)(47)(13629)$

4.2 Explicit Enumeration: Complete Bipartite Graphs

We can also directly count $|G(m, n)|$. We know (e.g. from the OEIS entry A136126) that

$$\begin{aligned}
|T(m+n, m)| &= \sum_{i=1}^{m+1} (-1)^{m+1-i} \cdot i! \cdot i^{n-1} \cdot S(m+1, i) \\
&= \sum_{i=1}^{n} (-1)^{n-i} \cdot i! \cdot i^{m} \cdot S(n, i) \\
&= n! n^m - \sum_{j=1}^{n-1} (-1)^{j-1} \cdot (n-j)! \cdot (n-j)^m \cdot S(n, n-j)
\end{aligned}$$

where the second equality follows from the symmetry $T(m+n, m) = T(m+n, n-1)$ (which itself isn't immediately obvious), and the third follows by pulling out the largest term of the sum, then reversing the order of summation. To prove this formula directly for $|G(m, n)|$, we will need a lemma:

Lemma 4.2.1. Fix $j < n$. The number of ways to partition $[n]$ into $n-j$ non-empty consecutive parts, then label all of the elements so that the labels within a part are in reverse order is $(n-j)!S(n, n-j)$. In other words, t is equal to the number of surjections from $[n]$ to $[n-j]$.

By consecutive, we mean the part contains all elements between its minimal and maximal part. e.g.

[123][45][6][78] is valid, [124][3] is not

Proof. Consider a surjection $g\colon [n] \to [n-j]$. The size of the preimage of each $i \in [n-j]$ gives the size of the ith part. e.g. if $|g^{-1}(1)| = 4$, then [1234] is a part. Surjectivity ensures each part is nonempty.

Then, simply label the elements from that part with the elements from the preimage in reverse order. e.g. if $g^{-1}(1) = \{4, 5, 7, 9\}$, then there would be a part [1234] with labels 9754 (in that order).

Going from the partition/labeling to a surjection g is done simply by letting the labeling of the first part be the preimage of 1, that of the second part be the preimage of 2, ... Nonempty parts ensures a surjective function. □

Theorem 4.2.2.

$$|G(m, n)| = n!n^m - \sum_{j=1}^{n-1} (-1)^{j-1} \cdot (n-j)! \cdot (n-j)^m \cdot S(n, n-j)$$

Proof. Consider the graph $K'_{m,n}$, the complete bipartite graph with m labeled vertices $L = \{1, \ldots, m\}$, and n unlabeled vertices $R = \{r, \ldots, r\}$.

Counting the number of AOs on $K'_{m,n}$ such that there are no sinks in L can be done by counting canonical topological sorts of the vertices such that the final vertex in the sort is from R. To do this, first write out all n vertices from R. Then, for each $v \in L$, v can be placed in any of the n spaces between these vertices (not counting the final space, since we don't allow v to be a sink).

Once such a space is chosen, v's ordering with respect to the other vertices of L in the same space is uniquely determined, since we are counting canonical sorts. Thus, we have n^m such acyclic orientations of $K'_{m,n}$.

$$\_r\_r\_r\_r \quad \longrightarrow \quad r13r2r4r$$

Now, we want to relabel the vertices of R, and count the resulting number of canonical topological sorts for $K_{m,n}$. For a given canonical topological sort of $K'_{m,n}$, there are $n!$ ways to relabel R, but some may result in a non-canonical sort.

Given any sort $\mathcal{O}$ for $K'_{m,n}$, we may refer to the ith occurrence of r as r_i, and for a particular relabeling ℓ, the corresponding label is $\ell(r_i)$. Also, say that $r_i \sim r_{i+1}$ denotes that they are adjacent in the sort (i.e. no vertex from L was placed in the space between them). Then, we may count the non-canonical sort/relabeling pairs as the union of sets:

$$A_i = \{(\mathcal{O}, \ell) \mid r_i \sim r_{i+1} \text{ and } \ell(r_i) > \ell(r_{i+1})\}$$

for each $i = 1, \ldots, n-1$ (it is clear that every non-canonical sort/relabeling pair must be in at least one such set). Then, inclusion-exclusion gives:

$$\left|\bigcup_{i=1}^{n-1} A_i\right| = \sum_{\varnothing \neq J \subseteq [n-1]} (-1)^{|J|-1} \left|\bigcap_{i \in J} A_i\right| = \sum_{j=1}^{n-1} (-1)^{j-1} \sum_{\substack{J \subseteq [n-1] \\ |J| = j}} \left|\bigcap_{i \in J} A_i\right|$$

For fixed J, $\left|\bigcap_{i \in J} A_i\right|$ is the number of sort/label pairs such that for each $i \in J$, $r_i \sim r_{i+1}$, and within a group of indistinguishable vertices, the relabeling is in reverse order (by definition of A_i). In particular, for a fixed j, we would like to count all of the ways to partition $r_1, \ldots, r_n$ into $n-j$ consecutive parts (this is the choice of J), then label them so that within each part the labelling is in reverse order. Notice, this is exactly what Lemma 4.2.1 counts. Then, after choosing a J of size j and the labels for the r_i, we must complete the orientation by choosing the placement of vertices from L. There are j spaces disallowed for placement of vertices from L, so there are $(n-j)^m$ choices of for each J. In total, we get that

$$\sum_{\substack{J \subseteq [n-1] \\ |J| = j}} \left|\bigcap_{i \in J} A_i\right| = (n-j)^m (n-j)! S(n, n-j)$$

and therefore

$$\left|\bigcup_{i=1}^{n-1} A_i\right| = \sum_{j=1}^{n-1} (-1)^{j-1} (n-j)^m (n-j)! S(n, n-j).$$

Finally, as these are the non-canonical sort/labelling pairs, we subtract from the total number to get the canonical ones

$$|G(m,n)| = n! n^m - \left|\bigcup_{i=1}^{n-1} A_i\right| = n! n^m - \sum_{j=1}^{n-1} (-1)^{j-1} \cdot (n-j)! \cdot (n-j)^m \cdot S(n, n-j)\,. \qquad \square$$

4.3 Explicit Enumeration: Complete Multipartite Graphs

Lemma 4.3.1. Consider the complete N-partite graph $K'_{n_1,\ldots,n_N}$ with the vertices in each $n_2, \ldots, n_N$-set unlabeled within their vertex set (we refer to these as $B, \ldots, Z$, and the labeled n_1-set as A). Then

$$\left|\mathcal{A}(K'_{n_1,\ldots,n_N})\right| = \left(1 + \sum_{i=2}^{N} n_i\right)^{n_1} \cdot \binom{\sum_{i=2}^{N} n_i}{n_2, \ldots, n_N}$$

Proof. We will count ways to construct an acyclic orientation of $K'_{n_1,\ldots,n_N}$ by first orienting edges disjoint from A, then orienting all edges containing a vertex from A.

To orient edges disjoint from A, we pick the topological sorting of vertices in $B \cup \ldots \cup Z$. Since these vertices are unlabeled (within their respective vertex sets), we can write a topological sort as a sequence containing n_2 b's, n_3 c's, ..., n_N z's. The number of such sequences is given by the multinomial coefficient

$$\binom{\sum_{i=2}^{N} n_i}{n_2, \ldots, n_N}$$

Next, to pick the orientations for the edges containing vertices in A, we simply pick where to insert each vertex $a_1, \ldots, a_{n_1} \in A$ into the topo-sort. There are $1 + \sum_{i=2}^{N} n_i$ 'slots' in the topo-sort (including the slot before all vertices and after all vertices). Notice that if two a_i, a_j get placed in the same slot, then their order within that slot does not matter – the resulting orientation is identical. So, we simply choose the slot of each vertex in A, with

$$\left(1 + \sum_{i=2}^{N} n_i\right)^{n_1}$$

choices.

In both steps, it is clear that the choice uniquely defines the orientations of the corresponding edges, and that the resulting orientation will be acyclic (since a topo-sort exists). Moreover, it is easy to see that any acyclic orientation of $K'_{n_1,\ldots,n_N}$ can be reached by such a construction. $\square$

Remark. Notice that we could easily alter this proof to count acyclic orientations of $K'_{n_1,\ldots,n_N}$ such that there are no sinks in vertex set A. The only modification needed is to disallow placement of vertices from A in the rightmost slot of the topo-sort. This means that there are only

$$\sum_{i=2}^{N} n_i$$

choices for each $a \in A$, which gives the total number of such acyclic orientations as

$$\left(\sum_{i=2}^{N} n_i\right) \cdot \binom{\sum_{i=2}^{N} n_i}{n_2, \ldots, n_N}$$

This will allow us to easily count the number of acyclic orientation with unique sink of multipartite graphs as well.

Remark. After choosing a particular acyclic orientation of $K'_{n_1,\ldots,n_N}$ we may order the vertices in each unlabeled set by its placement in the topo-sort, then refer to them in this order. This allows us to label these vertices, and refer to a particular vertex's label as e.g. $\ell(b_1)$.

Theorem 4.3.2. The number of acyclic orientations of the complete N-partite graph $K_{n_1,\ldots,n_N}$ is given by

$$|\mathcal{A}(K_{n_1,\ldots,n_N})| = \sum_{(k_2,\ldots,k_N)\in\mathcal{K}} \left((-1)^{\sum_{i=2}^N (n_i-k_i)} \cdot \left(1+\sum_{i=2}^N k_i\right)^{n_1} \cdot \binom{\sum_{i=2}^N k_i}{k_2,\ldots,k_N} \cdot \prod_{i=2}^N k_i! S(n_i,k_i) \right)$$

where $\mathcal{K} = [n_2] \times [n_3] \times \ldots \times [n_N]$.

Proof. First, we write an equivalent formula by reversing the order of summation along each $[n_i]$. Let $\mathcal{J} = \{0,\ldots,n_2-1\} \times \ldots \times \{0,\ldots,n_N-1\}$, and make the substitutions $j_i = n_i - k_i$. Then we will instead show that $|\mathcal{A}(K_{n_1,\ldots,n_N})|$ is given by

$$\sum_{(j_2,\ldots,j_N)\in\mathcal{J}} (-1)^{\sum_{i=2}^N j_i} \cdot \left(1+\sum_{i=2}^N (n_i-j_i)\right)^{n_1} \cdot \binom{\sum_{i=2}^N (n_i-j_i)}{n_2-j_2,\ldots,n_N-j_N} \cdot \prod_{i=2}^N (n_i-j_i)! S(n_i,n_i-j_i)$$

Lemma 4.3.1 gives a way to count $\left|\mathcal{A}(K'_{n_1,\ldots,n_N})\right|$, and we may consider all *relabelings* of vertices in sets $B,\ldots,Z$. There are $\prod_{i=2}^N n_i!$ such relabelings, and this gives a multiset $\mathscr{A}$ of acyclic orientations of $K_{n_1,\ldots,n_N}$ of size

$$|\mathscr{A}| = \left|\mathcal{A}(K'_{n_1,\ldots,n_N})\right| \cdot \prod_{i=2}^N n_i! = \left(1+\sum_{i=2}^N n_i\right)^{n_1} \cdot \binom{\sum_{i=2}^N n_i}{n_2,\ldots,n_N} \cdot \prod_{i=2}^N n_i!$$

If we denote the set of all relabelings as $\mathcal{L}$, then there is an obvious correspondence between $\mathscr{A}$ and $\mathcal{A}(K'_{n_1,\ldots,n_N}) \times \mathcal{L}$. It is also clear that eliminating duplicates in the multiset would exactly yield $\mathcal{A}(K_{n_1,\ldots,n_N})$. In particular, we can eliminate the non-canonical topological sorts.

A duplicate occurs when two different relabelings result in the same orientation (i.e. the only differences in the relabelings are in the labels of 'equivalent' vertices: those which have the same out-neighborhoods). To count duplicates, we define a canonical relabeling as having the labels of equivalent vertices be in-order with respect to the predefined ordering on these vertices (see the remark above).

That is, if for some particular orientation we have $b_i \sim b_j$ (they are equivalent) with $i < j$, then a canonical relabeling must have $\ell(b_i) < \ell(b_j)$. (And the same for C, D, ..., Z). Notice that since the predefined ordering is by topo-sort, two vertices can only be equivalent if they are either adjacent, or all vertices between them in the topo-sort are from the same vertex set (and thus also equivalent to them).

Thus, define the 'bad' sets for each vertex set $\mathcal{V} \in \{B,\ldots,Z\}$ and each vertex $v_i \in \mathcal{V}$ as containing a non-canonical adjacent pair:

$$\mathscr{B}_{\mathcal{V},i} = \{(\mathcal{O},\ell) \in \mathcal{A}(K'_{n_1,\ldots,n_N}) \times \mathcal{L} \mid v_i \sim v_{i+1}, \ell(v_i) > \ell(v_{i+1})\}$$

The non-canonical orientation/labeling pairs are counted as the union of these sets. Let

$$\mathcal{I} = \bigcup_{i=2}^N \{(V_i,k) \mid 1 \leqslant k < n_i\}$$

Using the principle of inclusion exclusion the number of non-canonical pairs is

$$\sum_{\varnothing \neq J \subseteq \mathcal{I}} (-1)^{|J|-1} \left| \bigcap_{(V,i)\in J} \mathscr{B}_{V,i} \right|$$

As with the previous theorem, we first consider all J such that j_2 pairs in B are equivalent, j_3 pairs in C are equivalent, ..., j_N pairs in Z are equivalent for some fixed $j_2, \ldots, j_N$. We can look at each vertex set independently and use Lemma 4.2.1 to see that in total, the number of ways to choose j_i indices in vertex set V_i and relabel to get get something in $\bigcap_{(V,i)\in J} \mathscr{B}_{V,i}$ is

$$\prod_{i=2}^{N} (n_i - j_i)! S(n_i, n_i - j_i).$$

Then, for each such J, regardless of the indices and labelling, the number of topological sorts can be counted identically to Lemma 4.3.1. This gives

$$\left(1 + \sum_{i=2}^{N} (n_i - j_i)\right)^{n_1} \cdot \binom{\sum_{i=2}^{N} (n_i - j_i)}{n_2 - j_2, \ldots, n_N - j_N}$$

ways. Therefore, if for $J \subseteq \mathcal{I}$, we denote $J_i = J \cap \{(V_i, k) \mid 1 \leqslant k < n_i\}$, then for any fixed $j_2, \ldots, j_N$,

$$\sum_{\substack{J \subseteq I \\ |J_i| = j_i}} \left| \bigcap_{(V,i)\in J} \mathscr{B}_{V,i} \right| = \left(1 + \sum_{i=2}^{N} (n_i - j_i)\right)^{n_1} \cdot \binom{\sum_{i=2}^{N} (n_i - j_i)}{n_2 - j_2, \ldots, n_N - j_N} \prod_{i=2}^{N} (n_i - j_i)! S(n_i, n_i - j_i).$$

This lets us rewrite the inclusion-exclusion as

$$\sum_{(j_2,\ldots,j_N)\in \mathcal{J}'} (-1)^{\left(\sum_{i=2}^{N} j_i\right)-1} \cdot \left(1 + \sum_{i=2}^{N} (n_i - j_i)\right)^{n_1} \cdot \binom{\sum_{i=2}^{N} (n_i - j_i)}{n_2 - j_2, \ldots, n_N - j_N} \cdot \prod_{i=2}^{N} (n_i - j_i)! S(n_i, n_i - j_i)$$

and subtracting this from $|\mathscr{A}|$, we get the desired result. □

Corollary 4.3.3. The number of acyclic orientations of the complete tripartite graph is given by

$$|\mathcal{A}(K_{m,k,n})| =$$
$$\sum_{i=0}^{k-1} \sum_{j=0}^{n-1} (-1)^{i+j} \cdot ((k-i) + (n-j) + 1)^m \cdot \binom{(k-i) + (n-j)}{n-j} \cdot (k-i)! S(k, k-i) \cdot (n-j)! S(n, n-j)$$

or, by substituting $s = k - i$ and $t = n - j$ in the sums:

$$|\mathcal{A}(K_{m,k,n})| = \sum_{s=1}^{k} \sum_{t=1}^{n} (-1)^{k+n-s-t} \cdot (s + t + 1)^m \cdot \binom{s+t}{t} \cdot s! S(k, s) \cdot t! S(n, t)$$

Theorem 4.3.4. The number of acyclic orientations with unique sink of $K_{n_1+1,n_2,\ldots,n_N}$ is given by

$$|\mathcal{A}(K_{n_1+1,n_2,\ldots,n_N}, q)| = \sum_{(k_2,\ldots,k_N)\in\mathcal{K}} \left((-1)^{\sum_{i=2}^N (n_i-k_i)} \cdot \left(\sum_{i=2}^N k_i\right)^{n_1} \cdot \binom{\sum_{i=2}^N k_i}{k_2,\ldots,k_N} \cdot \prod_{i=2}^N k_i! S(n_i,k_i) \right)$$

Proof. The proof is identical by just counting the number of acyclic orientations of $K_{n_1,\ldots,n_N}$ which have no sinks in A, and using the remark after Lemma 4.3.1. □

5 Extremal Problems

We are also interested in answering the following question: given a fixed number n of vertices, and m of edges, which graph(s) maximize the number of AOs?

It is conjectured by Cameron, Glass, and Schumacher that Turán graphs with two parts maximize the number of AOs over graphs with the same number of vertices and edges [CGS14]. We prove that Turán graphs with parts of size at most 2 are also maximizers.

Lemma 5.1. Let G be any graph containing edge $e = (a, b)$ such that

$$N(a) \setminus \{b\} \supseteq N(b) \setminus \{a\}$$

Then, for any edge $e' = (c, b) \notin E(G)$, $|\mathcal{A}(G)| \leqslant |\mathcal{A}(G \setminus e + e')|$.

Proof. Let $G' = G \setminus e + e'$. We know by the deletion-contraction recurrence for AOs that $|\mathcal{A}(G)| = |\mathcal{A}(G \setminus e)| + |\mathcal{A}(G/e)|$ (equiv. for G' and e'). Notice that clearly $G \setminus e = G' \setminus e'$ by our definition of G'.

Moreover, $G/e \cong G \setminus \{b\}$, since the new vertex ab resulting from contracting $e = (a, b)$ has neighborhood

$$N(ab) = (N(a) \setminus \{b\}) \cup (N(b) \setminus \{a\}) = N(a) \setminus \{b\}$$

while the rest of G is unchanged. On the other hand, G'/e' has new vertex bc resulting from contracting $e' = (c, b)$ with neighborhood

$$N(bc) = (N(b) \setminus \{c\}) \cup (N(c) \setminus \{b\}) \supseteq N(c) \setminus \{b\}$$

Therefore, $G'/e' \supseteq G \setminus \{b\}$, as the neighborhood of bc is no smaller than that of c. But

$$G/e \subseteq G'/e' \implies |\mathcal{A}(G/e)| \leqslant |\mathcal{A}(G'/e')| \implies |\mathcal{A}(G)| \leqslant |\mathcal{A}(G')| \qquad \square$$

Theorem 5.1. For $m \geqslant \binom{n}{2} - \left\lfloor \frac{n}{2} \right\rfloor$, the graph whose complement is a matching maximizes the number of AOs over all graphs on the same number of vertices and edges.

Proof. Lemma 5.1 can be interpreted in the complement: if there is an edge $e = (c, b)$ in $\overline{G}$, and a vertex a with $N(a) \subseteq N(b)$, then we can replace e with $e' = (a, b)$ in the complement without decreasing the number of AOs in G.

In particular, if a is an isolated vertex, we can always slide any edge to a. If there are at most $\left\lfloor \frac{n}{2} \right\rfloor$ edges in the complement and it is not a matching, then it has an isolated vertex. So for any graph whose complement is not a matching, there is a series of edge slides which don't decrease the number of AOs, and result in a graph whose complement is a matching. $\square$

Remark. Note that the complement of a matching is a Turán graph with parts of sizes 1 and 2.

6 Markov Chains and Hyperplane Arrangements

6.1 Background

Definition 6.1 (Hyperplane arrangement)**.** In real (affine) space $\mathbb{R}^n$, a **hyperplane arrangement** is a finite set $\mathscr{H}$ of hyperplanes in space. The **chambers** of a hyperplane arrangement are the connected components in $\mathbb{R}^n \setminus (\bigcup_{H \in \mathscr{H}} H)$.

Taking the intersection W of any number of hyperplanes in $\mathscr{H}$, restricting to W gives another hyperplane arrangement contained in W. The chambers of any such arrangements are called the **faces** of $\mathscr{H}$ (note, the chambers of $\mathscr{H}$ are faces of dimension n). Denote by $\mathcal{C}_{\mathscr{H}}$ and $\mathcal{F}_{\mathscr{H}}$ the set of chambers and faces of $\mathscr{H}$ respectively.

If we write $\mathscr{H} = \{H_1, \ldots, H_k\}$ and decide on a positive and negative side for each hyperplane, then a chamber C may be identified by its **sign sequence** $\sigma(C) = (\sigma_1, \ldots, \sigma_k)$, where $\sigma_i \in \{+1, -1\}$ depends on which side of H_i the chamber C lies on. Likewise, arbitrary faces have a unique sign sequence which identifies them, where $\sigma_i \in \{+1, 0, -1\}$. Any point in $\mathbb{R}^n$ also has a sign sequence, and it is the same as that of the unique smallest face containing that point.

Definition 6.2 (Face Semi-group)**.** We can define an operation of the faces $\mathcal{F}_{\mathscr{H}}$ as follows: for faces $F, G \in \mathcal{F}_{\mathscr{H}}$, define the **projection** FG of G on F as the face obtained by taking arbitrary points $f \in F$ and $g \in G$, and moving a small distance along the line from f to g. Equivalently, FG can be defined by its sign vector:

$$\sigma_i(FG) = \begin{cases} \sigma_i(F) & \text{if } \sigma_i(F) \neq 0 \\ \sigma_i(G) & \text{if } \sigma_i(F) = 0 \end{cases}$$

In particular, for a chamber C, FC is another chamber (since no entry in the sign vector can be 0).

A number of papers have considered and analyzed *Markov chains* on the chambers and faces of such hyperplane arrangements. This is of interest to us because of the following correspondence given by Greene and Zaslavsky [GZ83]:

Lemma 6.1.1. For a graph G on n vertices, the **graphical arrangement** is the hyperplane arrangement in $\mathbb{R}^n$

$$\mathscr{H}[G] = \{h_{ij} \mid \{i, j\} \in E(G)\}$$

where h_{ij} is the hyperplane $\{x_i = x_j\}$ defined by edge $\{i, j\}$. That is, the hyperplanes of $\mathscr{H}[G]$ correspond exactly to the edges of G. Moreover, we say that face F has sign vector σ such that for each edge $\{i, j\}$ with $i < j$, $\sigma_{ij}(F) = +1$ if the points in F satisfy $x_i < x_j$, and $\sigma_{ij}(F) = -1$ if $x_i > x_j$ (and as usual, $\sigma_{ij}(F) = 0$ if F lies on the corresponding hyperplane). Then, there is a bijection between the acyclic orientations of G and the chambers of $\mathscr{H}[G]$ given by:

- A given orientation $\mathcal{O}$ corresponds to the chamber with sign sequence $\sigma_{ij} = +1$ if edge $\{i, j\}$ is oriented as $i \to j$ in $\mathcal{O}$, and $\sigma_{ij} = -1$ if it is oriented in the other direction.
- Given a chamber C, orient edge $\{i, j\}$ as $i \to j$ if $\sigma_{ij}(C) = +1$, and $j \to i$ if $\sigma_{ij}(C) = -1$.

In other words, we may talk about the chambers of a graphical hyperplane arrangement interchangeably with the acyclic orientations of the corresponding graph. Next we will discuss Markov chains on hyperplane arrangements, for which we must first cover the necessary terminology. More details of the following discussion can be found in any introduction to Markov chains, such as the textbook by Levin and Peres [LP17].

Definition 6.3 (Markov chain)**.** A finite **Markov chain** is a sequence of discrete random variables $X_1, X_2, \ldots$, each taking values from finite **state space** Ω, such that for every t, and every $x_1, \ldots, x_t \in \Omega$,

$$\Pr\left[X_t = x_t \mid X_1 = x_1, \ldots, X_{t-1} = x_{t-1}\right] = \Pr\left[X_t = x_t \mid X_{t-1} = x_{t-1}\right].$$

We call the Markov chain **time-invariant** if the distribution $\Pr\left[X_t \mid X_{t-1}\right]$ doesn't depend on t. In this case, we can associate a **transition matrix** K with the Markov chain of size $|\Omega| \times |\Omega|$, and indexed by elements of Ω such that for every $x, y \in \Omega$,

$$\Pr\left[X_t = y \mid X_{t-1} = x\right] = K(x, y).$$

Given a distribution μ_t over the state space at time step t, the language of Markov chains allows us to determine the distribution μ_{t+1} by treating these distributions as row vectors. Then $\mu_{t+1} = \mu_t K$. More carefully,

$$\mu_{t+1}(y) = \Pr\left[X_{t+1} = y\right] = \sum_{x \in \Omega} \Pr\left[X_t = x\right] \Pr\left[X_{t+1} = y \mid X_t = x\right] = \sum_{x \in \Omega} \mu_t(x) K(x, y).$$

Definition 6.4 (Stationary Distribution)**.** For a finite Markov chain with state space Ω and transition matrix K, a stationary distribution π is a distribution over the state space such that

$$\pi K = \pi.$$

There are a number of classical results on Markov chains and their convergence to a stationary distribution. In particular, if a Markov chain is *irreducible* and *aperiodic*, then it has a unique stationary distribution π. Moreover, the Convergence Theorem says that given any starting distribution μ_0, the distribution $\mu_t = \mu_0 K^t$ will eventually converge to π:

$$\left\|\mu_0 K^t - \pi\right\|_{TV} \to 0$$

where the norm is the *total variation distance.*

The main idea in Markov chain Monte Carlo techniques is that we have a space Ω which we would like to sample from (e.g. acyclic orientations of a graph, or chambers of a hyperplane arrangement). We design a Markov chain (formally, a family of Markov chains. One for each instance, e.g. each graph or hyperplane arrangement) on the state space such that the stationary distribution is our desired sampling distribution. Then the Convergence Theorem says that by starting at an arbitrary state and *simulating* the Markov chain, after sufficiently many time steps the state will be chosen approximately from our desired distribution.

In order for this scheme to be effective, we have to ensure that the Markov chain can be simulated efficiently, and that the time of convergence is small (polynomial) in terms of the size of the input (e.g. size of the graph, number of hyperplanes).

We now introduce a Markov chain on the chambers of a general hyperplane arrangement discussed and analyzed by Brown and Diaconis [BD98]. Given a hyperplane arrangement $\mathscr{H}$, let the state space be $\Omega = \mathcal{C}_{\mathscr{H}}$. Let w be some distribution over $\mathcal{F}_{\mathscr{H}}$. Then, define the transition from any state $C \in \Omega$ as

1. Choose a random face F via the distribution w.

2. Move from C to the projection FC.

Equivalently, the transition matrix is defined as

$$K(C, C') = \sum_{\substack{F \in \mathcal{F}_{\mathscr{H}} \\ C' = FC}} w(F).$$

Theorem 6.1.2 ([BD98])**.** For the Markov chain on chambers described above,

1. K has eigenvalues associated with intersections of hyperplanes. For each intersection W of some hyperplanes, there is an eigenvalue

   $$\lambda_W = \sum_{\substack{F \in \mathcal{F}_{\mathscr{H}} \\ F \subseteq W}} w(F) \quad \text{with multiplicity} \quad m_W = |\mu(\mathbb{R}^n, W)|$$

   where μ is the *Möbius function* of the poset of intersections of hyperplanes ordered by reverse inclusion (so $\mathbb{R}^n$ is the least element).

2. K has a unique stationary distribution π if and only if w is *separating*. That is, if the faces in the support of w (those with non-zero probability) do not all lie on a single hyperplane.

3. If w is separating, then we have the following characterization of the stationary distribution π: by sampling from w without replacement we get a sequence $F_1, \ldots, F_m$ of all of the faces in the support of w. Taking the projection in the face semi-group of this sequence gives a chamber $C = F_1 F_2 \ldots F_m$ which is distributed as π.

Athanasiadis and Diaconis noticed that this general Markov chain can be used to consider several Markov chains on the acyclic orientations of a graph [AD10]. In particular, for graph

G they considered the Markov chain on the chambers of $\mathscr{H}[G]$ defined by w being the uniform distribution over all faces F_v for $v \in G$ a vertex, where

$$\sigma_{ij}(F_v) = \begin{cases} -1 & \text{if } i = v \\ +1 & \text{if } j = v \\ 0 & \text{otherwise} \end{cases}$$

for all edges i, j in G (with $i < j$). Notice that every graphical arrangement contains a face with such a sign sequence since, in particular, the point $x = (0, \ldots, 1, \ldots, 0) \in \mathbb{R}^m$, where the 1 is at coordinate x_v, has this sign sequence: $x_v > x_i$ for all i, and $x_i = x_j$ when $i, j \neq v$. Now notice by the correspondence between sign sequences in graphical arrangements and orientations of of the graph: this is exactly equivalent to the Markov chain on AOs of G in which a random vertex is chosen, and all edges incident to that vertex are oriented toward it. While this particular choice of w gives a Markov chain with a simple interpretation in terms of G, other choices of w could give less natural Markov chains on AOs.

Finally, Billera, Brown, and Diaconis considered this walk on 3-dimensional arrangements [BBD99]. They found

Theorem 6.1.3 ([BBD99])**.** Consider $\mathscr{H}$, an arrangement of m hyperplanes in $\mathbb{R}^3$ whose intersection is $\{0\}$. Let w be uniform over the 1-dimensional faces of $\mathscr{H}$, and consider the corresponding Markov chain. Then for any chamber C with i sides (e.g. a slice of the chamber is a polygon with i faces), the stationary distribution π satisfies

$$\pi(C) \propto i - 2$$

In particular, the probability of a chamber depends only on the "shape" of the chamber.

6.2 A Specific Markov Chain

It is not hard to see that a k-dimensional face in a graphical arrangement $\mathscr{H}[G]$ corresponds to a partition of the vertices into k sets $V_1, \ldots, V_k$ such that the induced subgraph on each V_i is connected, and an acyclic orientation on the meta-graph formed by collapsing each part into a single vertex. In particular, 2-dimensional faces are cuts $(S, \overline{S})$ in the graph such that the two parts are connected subgraphs, and the edges between them are oriented all from either $S \to \overline{S}$ or $\overline{S} \to S$.

Any graphical arrangement $\mathscr{H}[G]$ contains only hyperplanes of the form $x_i = x_j$. Therefore, every hyperplane in the arrangements contains the line $x_1 = x_2 = \ldots = x_n$. Thus, the space in a graphical arrangement can be modded out along this line to yield an equivalent hyperplane arrangement whose faces are one dimension smaller. As this is a simplification for graphical arrangement, we will consider $\mathscr{H}[G]$ to be this lower dimensional arrangement.

Now, on the simplified graphical arrangement $\mathscr{H}[G]$, the 2-dimensional faces discussed above correspond to 1-dimensional faces. We consider the arrangement walk on the simplified arrangement defined by letting the distribution w be uniform on the 1-dimensional faces. In graphical language, this is a walk on AOs with a step:

1. Pick uniformly at random from the set of cuts $(S, \overline{S})$ in the graph such that both parts are connected subgraphs.

2. Pick uniformly a direction $S \to \overline{S}$ or $\overline{S} \to S$.

3. Orient all edges between S and $\overline{S}$ with direction determined by step 2.

We plan to analyze this Markov chain, in particular hoping to address some or all of the following questions:

1. Notice that when the number of vertices $n = 4$, then the simplified arrangement is 3-dimensional, and satisfies the criteria of the result on 3-dimensional arrangements by Billera, Brown, and Diaconis [BBD99]. In particular, the probability of an AO in the stationary distribution depends only on the shape of the corresponding chamber.

   Experimentally, it appears the same statement holds true for more vertices, though it is not clear what the dependence might be. In particular, we would like to determine if the the probability of an AO depends on the f-vector of the cross-section of the corresponding chamber, or the combinatorial type of the cross-section (or neither).

2. We want to be able to sample AOs uniformly, but the stationary distribution is not uniform. There are ways to get around this (i.e. Metropolis filter), but the most basic way applies only when the Markov chain is *time reversible*. This one is not in general, see Example 6.2.2 below. Is there some other way to alter the chain and make it uniform?

3. It is not immediately clear how to efficiently simulate this Markov chain. We would like to determine if there is an efficient way to uniformly sample a connected subset of vertices with connected complement. Simple rejection sampling doesn't work in general, since the number of such subsets could be exponentially small compared to the total number of subsets of vertices. See Example 6.2.1 below.

4. It is not known what the *mixing time* (i.e. the time until approximate convergence to stationarity) of the Markov chain is. We would like to find a polynomial bound (in terms of the size of the graph) on the mixing time, if one exists.

Example 6.2.1 (Trees)**.** Consider this Markov chain on a tree $T = (V, E)$. First, notice that any connected subset $S \subsetneq V$ which isn't the entire tree has connected complement. Each such subset can be identified by the edge which spans the cut $(S, \overline{S})$. Therefore, in the case of trees, this Markov chain is simply choosing an edge uniformly at random, then an orientation for that edge uniformly at random.

We may make two observations about this special case:

- The Markov chain is symmetric. That is, $K(x, y) = K(y, x)$. This is clear, since either both are 0, or AOs x and y differ by a single edge's orientation. In the latter case, the probability of picking that edge and flipping its direction is the same from x as it is from y.

  Symmetry of the Markov chain implies that its stationary distribution π is uniform over all AOs (the desired distribution). We can see this by noticing that K being a stochastic matrix gives it a uniform right eigenvector, and so symmetric means the uniform distribution is also a left eigenvector, so $\pi K = \pi$.

- Rejection sampling does not work to find a connected subgraph S with connected complement. Indeed, we argued that there are only $m = n - 1$ such sets, since this is the number of edges in a tree. However, there are of course $2^n - 2$ non-empty subsets of vertices.

Note, however, that the sampling and counting problems for AOs on trees is trivial: all orientations are acyclic, so we can just sample a random orientation by orienting each edge independently. Moreover, there are always exactly $2^m = 2^{n-1}$ AOs.

Definition 6.2.1 (Time-reversible)**.** A Markov chain with transition matrix K is said to be **time-reversible** if the stationary distribution π satisfies

$$\pi(x)K(x, y) = \pi(y)K(y, x)$$

for all pairs of states x and y.

Example 6.2.2 (Complete Graphs)**.** On the complete graph K_n, AOs are in bijection with orderings/permutations of the vertices. A step in the Markov chain can then be interpreted as: start with an ordering $\sigma = v_1, \dots, v_n$ of the vertices. Then select a random subset to "move to the front" maintaining relative ordering. That is, select a random subset $S = \{v_{i_1}, \dots, v_{i_k}\}$ where $i_1 < i_2 < \ldots < i_k$, and let $\overline{S} = \{v_{j_1}, \dots, v_{j_{n-k}}\}$ where $j_1 < \ldots < j_{n-k}$. Then a step moves from σ to the permutation $\sigma' = v_{i_1}, \dots, v_{i_k}, v_{j_1}, \dots, v_{j_{n-k}}$.

We again make two observations:

- The Markov chain in this case *is not* symmetric. Indeed, if we consider K_4, then we can go from permutation $\sigma = 1234$ to $\sigma' = 2413$ by selecting $S = \{24\}$. However, no choice of S takes us from σ' to σ.

  In particular, we have $K(\sigma, \sigma') > 0$, while $K(\sigma', \sigma) = 0$. This not only rules out symmetry of the Markov chain; it also ensures that it is not time-reversible (assuming $\pi(\sigma) \neq 0$, which is clearly the case here).

- The stationary distribution π is still uniform, despite K not being symmetric. Indeed, for any two permutations σ_1, σ_2 on the vertices, there is a permutation η such that $\sigma_2\eta = \sigma_1$ (in particular, $\eta = \sigma_2^{-1}\sigma_1$). Then, it is not hard to see that for any permutation ν, $K(\nu, \sigma_1) = K(\nu\eta, \sigma_2)$. In particular,

  $$\sum_\nu K(\nu, \sigma_1) = \sum_\nu K(\nu\eta, \sigma_2) = \sum_\nu K(\nu, \sigma_2)$$

From here it is obvious that $\pi K = \pi$ for π equal to the uniform distribution.

As with trees, the sampling and counting problems for AOs on K_n is trivial: we know how to efficiently sample permutations, and there are $n!$ of them.

TODO: Determine if there is something nice I can say about cycles

7 Concluding Remarks

There are many questions in this area which are still open. We will list a few here, which may be worked on in the future.

1. We would primarily be interested in answering many of the questions raised in Section 6.2.

   In particular, regarding finding a Markov chain with uniform stationary distribution, we may consider the *time reversal* chain, with transition matrix defined by $K^*(x, y) = \frac{\pi(y)K(y,x)}{\pi(x)}$, which has the same stationary distribution. Then, there are a number of ways to form a new Markov chain which *is* time-reversible, and thus could be used in conjunction with a Metropolis filter to get a uniform distribution. For example,

   $$K' = \frac{K + K^*}{2}$$

   Notice that the definition of K^* depends on the ratio $\frac{\pi(y)}{\pi(x)}$ for x and y for which either $K(y, x)$ is non-zero. While it might be difficult to find a precise description of π, it is possible the ratio could have a simple description. Moreover, there are a number of Metropolis filters (e.g. [Cho20]), some of which may be computable only knowing the ratios of entries of the stationary distribution.

2. Postnikov found that the number of AOs of $K_{m,n}$ equals the number of placements of $m + n$ pairwise non-attacking rooks on a certain chess board. We wonder if there is a generalization of this to complete multipartite graphs.

3. It would be interesting to tighten the bounds on the number of AUSOs of the hypercube graph Q_d from what Matoušek was able to achieve. In particular, it is known that

   $$\frac{1}{2} \leqslant \frac{\log_2|\mathcal{A}(Q_d, \cdot)|}{2^d} \leqslant \log_2(d-1)$$

   It would be very interesting to determine if either $\frac{\log_2|\mathcal{A}(Q_d,\cdot)|}{2^d} = O(1)$, or $\frac{\log_2|\mathcal{A}(Q_d,\cdot)|}{2^d} = \Omega(\log d)$, or if the true answer lies somewhere in between.

4. It would be interesting to know whether the Turán graph is always a maximizer for the extremal problem of Section 5.

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